

Reconstruction of SAXS Data using Neural Networks

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We aim to simplify the process of reconstructing electron densities from SAXS images by employing a special Neural Network architecture, the conditional Invertible Neural Network (cINN). The only requirement is a simulation from electron density to diffraction image to generate a training dataset. Once trained, it can make accurate and fast (ms range) predictions on simulated and experimental data and furthermore resolve ambiguities resulting from the phase problem. Some challenges remain though, since we cannot differentiate between accurate predictions and false predictions from experimental data not covered by the training dataset (out-of-distribution data) as the output does not convey the degree of certainty of the prediction made by the cINN.

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